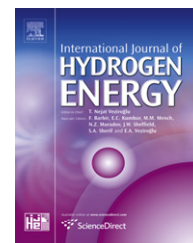


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Technical Communication

Direct injection of hydrogen, oxygen and water in a novel two stroke engine

Alberto Boretti^{a,b,*}, Azmi Osman^c, Ishak Aris^d

^a University of Ballarat, PO Box 663, Ballarat, 3353 VIC, Australia

^b Missouri University of Science and Technology, 194 Toomey Hall, Rolla, MO 65409-0050, United States

^c PROTON Holdings Berhad, HICOM Industrial Estate, Batu Tiga, 40000 Shah Alam, Selangor, Malaysia

^d Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia

ARTICLE INFO

Article history:

Received 1 April 2011

Received in revised form

6 May 2011

Accepted 7 May 2011

Available online 12 June 2011

Keywords:

Hydrogen internal combustion engines

Oxy-fuel combustion

Direct injection

Water injection

Exhaust energy recovery

Variable valve actuation

ABSTRACT

This short communication proposes novel two stroke engine burning hydrogen in oxygen in presence of large amounts of steam as residual gases. This engine has a bowl-in-piston combustion chamber, exhaust valves only and it uses direct injection of hydrogen, oxygen and water. Diesel-like compression ignition combustion is achieved by injecting the oxygen and the hydrogen in the surrounding steam close to a continuously operated glow plug. The operation of the engine is simulated by commercial softwares. The water injection enables acceptable metal temperatures and reduced heat losses. First computational results show brake efficiencies above 55% achieved with mass of water injected about twice the mass of oxygen and hydrogen mixture and operation with a significant amount of exhaust gas recirculation. It seems reasonable to guess efficiencies of the fully optimised and developed engine approaching the 60% mark, 20% higher than those of the state-of-the-art H₂ICEs designed for operation with air using the spark-ignition engine concept as well as of those projected for Diesel engines operating with exhaust energy recovery. Worth of mention is also the much higher power density following the two stroke operation.

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1. Introduction

Hydrogen fuel does not occur naturally on Earth and thus it is not an energy source but an energy carrier. Currently it is most frequently made from methane or other fossil fuels. However, it can be also produced from a wide range of renewable sources such as wind, solar or tides, that are intermittent too diffuse or too unwieldy to directly propel a vehicle, from the splitting of the water molecule. Integrated wind-to-hydrogen

plants using electrolysis of water are exploring technologies to deliver hydrogen with costs low enough and in quantities great enough to compete with traditional fuels.

In a future hydrogen economy, renewable hydrogen would be the product of the splitting of the water molecule through the use of renewable energy sources as wind, tides or solar and it might become the preferred transportation fuel. This splitting could make available not just the hydrogen, but also the oxygen required for combustion, being oxygen an

* Corresponding author. University of Ballarat, PO Box 663, Ballarat, 3353 VIC, Australia. Tel.: +61 3 5327 9108; fax: +61 3 5327 9240.

E-mail address: aboretti@staff.ballarat.edu.au (A. Boretti).

interesting by-product obtained with negligible additional costs.

In hypothesis to have hydrogen and oxygen readily available for an internal combustion engine, then it makes sense to explore the option to burn hydrogen in oxygen within an internal combustion engine that will operate free not only of carbon dioxide but also free of all the other pollutant emissions like HC, CO, NO_x and PM.

Oxygen and hydrogen in liquid form have been the preferred fuel and oxidizer for space propulsion. Liquid oxygen (LOX) and liquid hydrogen are the most common liquid propellants in use today. Hydrogen and oxygen are used to power space rockets since decades because they provide the largest amount of energy per unit mass of mixture of any fuel and oxidizer combination.

The internal combustion engine is the preferred engine for transport applications because of its simplicity, low cost and power density. Top fuel conversion efficiencies are now approaching 45% in passenger car applications and 50% in heavy duty truck applications. Stationary applications may provide even better efficiencies optimizing the low speed constant operation and better recovering the exhaust and the coolant and oil heat.

Many companies are working to develop engines that might efficiently exploit the potential of hydrogen. The attraction of using hydrogen as an energy carrier is that, if hydrogen is prepared without using fossil fuel inputs, vehicle propulsion would not contribute to carbon dioxide emissions and the depletion of fossil fuel resources. Furthermore, hydrogen engines will not emit pollutants with the only exception of NO_x when burned in air. Therefore, no global or local environmental impacts of transport solutions could be the major outcomes of hydrogen cars.

The idea to power cars with hydrogen fuelled engines is more than 200 years old. In 1807, François Isaac de Rivaz invented the hydrogen and oxygen powered internal combustion engine with electric ignition. In 1808 he fitted this engine into a working vehicle that is considered the world's first internal combustion engine powered automobile [1]. This engine was not a commercial success. Nevertheless, in 1863, Étienne Lenoir invented the Hippomobile, an automobile with a hydrogen gas-fuelled single cylinder internal combustion engine. Lenoir sold about 350–400 Hippomobiles [1], a success for the time. After these two experiences, the hydrogen engine did not received too much of attention until recently, possibly because other fuels – gasoline and Diesel – were permitting much better cost to benefit ratio as transportation fuels.

Apart from these two remarkable experiences of the past, the hydrogen internal combustion engine (H₂ICE) is a concept only recently introduced in demonstration vehicles built by Original Equipment Manufacturers (OEM), from the Mazda HR-X and MX-5 MiataHydrogen Wankel Rotary of the early 1990s to the BMW Hydrogen 7 and H₂R of the latest 2000s just to mention the most remarkable solutions, all of them starting from a gasoline-fuelled power plant, and all of them burning hydrogen in air.

The most part of the H₂ICEs proposed so far by engine researchers and OEM have been designed for operation gasoline-like. Many traditional gasoline engines have been modified for manifold or port injection of hydrogen running

lean of stoichiometry in air to avoid the abnormal combustion events of hydrogen with combustion controlled by a spark discharge and load controlled by throttling the intake. Direct injection of hydrogen has proved to be effective in improving the performances of these gasoline-like H₂ICEs [2]. Diesel-like applications have also been proposed by some researchers with manifold injection of small quantities of hydrogen in a traditional Diesel engine. These engines operate dual fuel Diesel and hydrogen. Results obtained so far have been less promising than in the gasoline-like applications. However, Diesel-like H₂ICEs with direct injection of hydrogen with or without the dual fuel operation are certainly an area worth of further investigation for the higher fuel conversion efficiencies both top and part load thanks to the advantages of the lean diffusion combustion and the load control by quantity of fuel injected. Auto ignition of hydrogen in air is possible in the presence of a continuously operated glow plug [3].

The state-of-the-art hydrogen engines for both gasoline-like and Diesel-like applications were assessed in two European projects of the latest 2000s. In the HyICE project [2] it was demonstrated that a gasoline-like hydrogen engine with spark-ignition and direct fuel injection may outperform current gasoline engines in terms of power density and efficiency. In the H₂BVplus project [11,12], the opportunity to design a Diesel-like engine was also investigated to demonstrate the advantages of the conventional Diesel-like compression ignition (CI) process compared with the Spark-Ignition (SI) process with a hydrogen engine. Although it was only possible to demonstrate pure auto ignition for non-automotive conditions, the H₂BVplus project showed the advantages of the Diesel principle using a continuously operated glow plug combustion system throughout the map at high efficiency levels.

This project further develops the Diesel-like combustion process in presence of a continuously operated glow plug. However, the direct injection of oxygen coupled to the direct injection of hydrogen makes the engine concept unique. The novel engine does not require intake valves, and may be therefore developed according to the two strokes rather than the four stroke principle for an increased power density. Direct water injection is finally also adopted to operate the engine with large amount of residuals to reduce the heat losses to the wall as well as to control the peak metal temperatures.

Water injection has been used since decades to control the occurrence of knock and the temperature of gases to turbine in spark ignited engines, and it has been recently proposed in [4] as an enabler of the stoichiometric operation of hydrogen fuelled direct injection spark-ignition engines.

2. Engine concept

Availability of high pressure oxygen and hydrogen and the recent advances in direct injection may permit the design of a novel engine that may burn hydrogen much more efficiently than in today's best four stroke engines having the power densities of today's best two stroke engines.

Hydrogen has an adiabatic flame temperature of 2483 K when it is burned in stoichiometric air in which for

combustion purposes may be assumed composed of 23.3% oxygen and 76.7% nitrogen (mass fractions). If air is replaced by oxygen only, the adiabatic flame temperature then rises up to 3473 K. At this high temperature, the temperature limits for common metals used in engine can normally be exceeded. Both mineral and synthetic engine oil have limited temperature range thus the risk of piston scuffing needs to be mitigated.

For an internal combustion engine, the only opportunity to keep the temperatures under control is to burn hydrogen and oxygen diluted in a large amount of residual gases and using water as a cooling agent that has high specific heat capacities and latent heat of evaporation. In this context the cooling agent is introduced in liquid state to enable it to effectively absorb the excess heat until it evaporates.

Hydrogen has a Lower Heating value of $1.20\text{E} + 08$ J/kg while water has a heat of vaporization at 298 K of $2.44\text{E} + 06$ J/kg. The heat released during combustion of 1 kg of hydrogen may therefore vaporise up to almost 50 kg of water. During combustion of hydrogen in stoichiometric oxygen, 9 kg of steam are formed from 1 kg of hydrogen and 8 kg of oxygen. Management of steam within the cylinder appears therefore the key factor in developing an internal combustion engine using oxygen and hydrogen. In addition to that, new kind of material and coating need to be considered for engine parts that are exposed to the extreme temperature inside the combustion chamber.

A two stroke engine is an internal combustion engine that completes the process cycle in one revolution of the crank shaft compared to twice that number for a four stroke engine. This is usually accomplished by using the beginning of the compression stroke and the end of the combustion stroke to perform simultaneously the intake and exhaust (scavenging). Two stroke engines are very well known to have power densities much higher than four stroke engines at least in a narrow range of rotations speeds but usually a much more complicated gas exchange process resulting in increased pollutants and reduced fuel conversion efficiency.

The manuscript describes the design of an engine for burning hydrogen in oxygen in a stoichiometric ratio. This engine has the advantages of the much faster combustion and the much larger energy available per unit mass of fuel and oxidizer as well as the ability to produce only steam as the product of combustion. The engine has water, oxygen and hydrogen injectors and two exhaust valves plus a central jet ignition device. The combustion chamber is made of a flat cylinder head and a bowl-in-piston as traditional in Direct Injection Diesel engines. The engine has a power turbine downstream connected to the crank shaft to supplement the torque produced by the piston work recovering part of the exhaust energy. Fully variable valve actuation is also adopted to better manage the steam within the cylinder. This engine concept is an original extension of the work proposed in [5]. Fig. 1 presents the combustion chamber layout and the full load operating principles of the oxy-fuel engine concept proposed there. In this case, the fuel is Diesel, and the engine is operating with the compression ignition principle. A glow plug not represented there is also needed to increase the cylinder temperature especially during the engine start up operation.

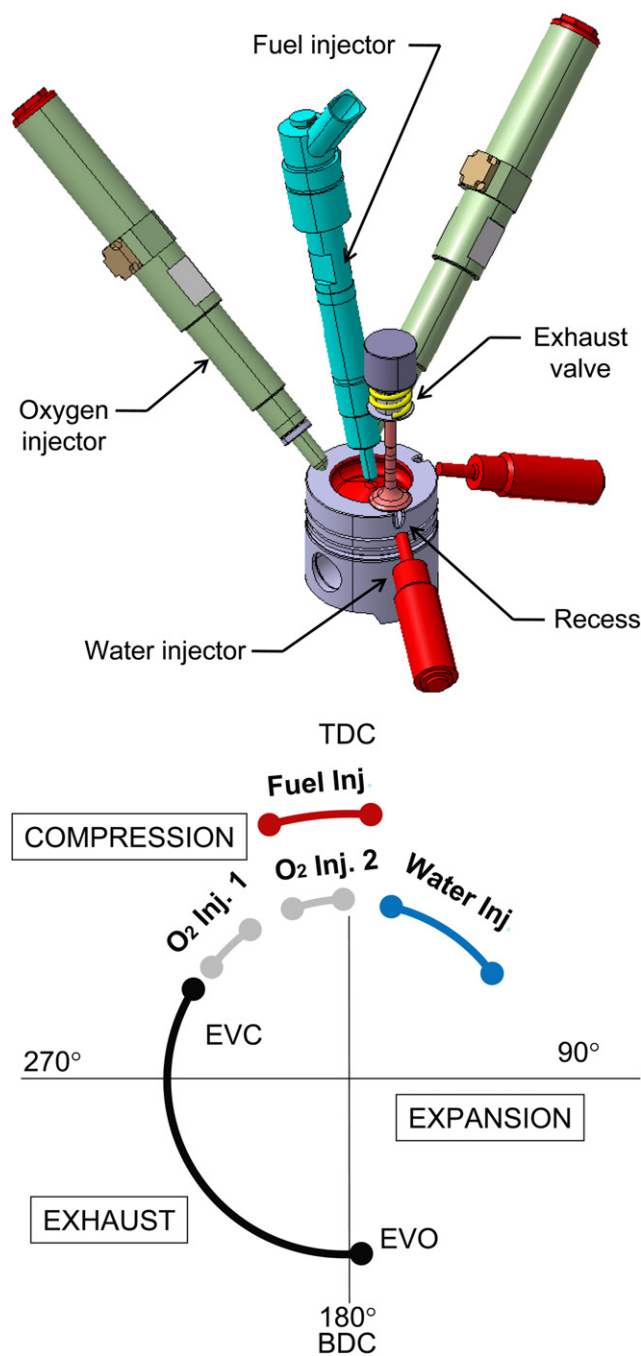


Fig. 1 – Combustion chamber layout and full load operating principles of the oxy-fuel engine concept proposed in [5].

The present application differs for the use of hydrogen replacing the Diesel fuel, the presence of the continuously operated glow plug, the injection of oxygen and hydrogen occurring later during the compression stroke and finally the injection of water later in the expansion stroke.

Hydrogen injectors are now available off-the-shelf from several manufacturers [6,7]. Direct Injectors for H_2 and CNG operates with inlet pressure up to 300 bar and permits short injection times, high temperature, high durability and dry run capability. At temperatures about 298 K and pressures about

300 bar, the density of hydrogen is about 20.546 kg/m^3 , while oxygen has a density of 392.68 kg/m^3 and methane a density of 212.81 kg/m^3 . Therefore, delivery of oxygen and hydrogen in stoichiometric ratio (8:1) is not an issue using off-the-shelf these high pressures H_2 and CNG injectors for both fluids, and possibly is the direct injection of water that may possibly pose more issues using Diesel or gasoline direct injectors for first prototyping.

About top dead centre, the engine receives in the central area surrounded by the bowl walls the incoming oxygen and hydrogen jets. The oxygen injection start first, and the hydrogen is injected in the oxygen. With high compression ratios, the cylinder pressure and temperatures are very high, especially when there is no injection of water and the amount of residuals is low, and the continuous operation of the glow plug may help to further reduce the auto ignition delay time.

Even if the option has not been investigated so far, the fully variable exhaust valve actuation may certainly also be used to change the effective compression ratio, the residual mass fraction and the temperature and pressure of the gases at the start of injection. As soon as the piston moves towards the bottom dead centre, water is injected to lower the in-cylinder temperature and to produce additional steam (steam is also the result of the hydrogen-oxygen combustion) that also expands within the cylinder. Even if the option has not been investigated so far, we may consider injecting the water early right after the fuel auto ignition occurs. Oxygen combustion normally produces intense heat release thus immediate cooling is a necessity.

Water injection may also be performed if necessary during compression, even if varying the effective compression ratio to control the cylinder temperature gives a much better impact if compared to water injection.

Approaching bottom dead centre, the exhaust valves then open and during the first half of the compression stroke the steam is partially evacuated from the in-cylinder. About halfway through the compression stroke, the exhaust valves close and the remaining steam is compressed while the piston is approaching the top dead centre position. Using the variable exhaust timing and lift to accurately control the cylinder temperature at the point of auto ignition is certainly an opportunity worth exploration currently neglected for sake of simplicity. The steam exiting the cylinder is further expanded in a power turbine directly connected to the crank shaft before it is exhausted in atmosphere. Because the product of combustion is just steam, no exhaust after treatment is necessary.

The fully variable operation of the exhaust valves, coupled to the direct water injection, enables control of the combustion evolution as well as of the temperature to the turbine at the different loads and speeds, while the amount of hydrogen and oxygen injected control the load for every speed. The power turbine downstream may possibly be by-passed when the exhaust energy recovery is less than the loss of energy due to the increased back pressure.

For car industry, it might certainly be difficult to force customers to have to control two or even three filling levels. However, the filling of the oxygen and hydrogen tanks is related since they must combine in stoichiometric ratio, and the water tank may possibly be at least partially refilled by

condensing the exhaust (some of the steam may escape and being discharged to the environment).

The wall heat losses due to very high temperatures and a small quenching distance are not an issue because the hydrogen and the oxygen are injected in the bulk of the combustion chamber surrounded by a large quantity of steam.

Glow plugs will certainly have higher demand on auxiliary energy than spark plugs. Glow plugs are certainly needed during cold start, and then when a large amount of water is injected and the temperature of gases within the cylinder will otherwise produce too long auto ignition times.

A few operating points have been considered so far. The turbine might need a CVT to crank shaft if the range of acceptable speeds of rotation of the turbine with a fixed ratio could be less than the range of speeds of the engine. However, two stroke engines are not expected to run over wide ranges of engine speeds and all the simulations below have been done with a fixed gear ratio.

The paper presents in the next section first results of simulations performed with well established computational fluid dynamic and engine performance simulation codes.

3. Results

Simulations have been performed by using STAR-CCM [8] and DARS [9] for the non premixed combustion of hydrogen in oxygen. Details of coupled STAR-CCM and DARS simulations of non premixed combustion of hydrogen in oxygen and nitrogen have been presented in [3]. As a first approximation, species considered are now only H_2 , O_2 , H , O , OH , HO_2 , H_2O , H_2O_2 (no N_2) and the 18 forward and backward steps of the H_2/O_2 kinetic mechanism is the one proposed in [3] with the forward and backward step involving N_2 in the table obviously deleted. These simulations of late compression and first expansion strokes with injection of oxygen and hydrogen show the opportunity to achieve a combustion Diesel-like, where the heat release rate is characterized by a chemically controlled ignition delay, followed by a premixed combustion where chemistry is still the controlling factor, and then finally by a diffusion combustion that is fully controlled by the mixing. The goal of the injection of oxygen and hydrogen in a high temperature environment controlled by the continuously operated glow plug in addition to the residual exhaust gases is the opportunity to achieve a fast combustion immediately after top dead centre.

An engine model has then been defined using the GT-POWER software [10]. GT-POWER is widely used in both the industry and the academy since more than two decades. It is very well documented and it has been extensively validated by the developer as well as by the users vs. reliable engine data generally providing satisfactory accuracy. In the model, three injectors introduce oxygen, hydrogen and water within the cylinder and two exhaust valves expel the combustion gases (steam) from the cylinder up to a power turbine where they further expand before being discharged in the atmosphere.

The engine cylinder has an 80 mm bore and an 80 mm stroke and a 145 mm connecting rod. The compression ratio is a $\text{CR} = 22:1$. This value has been selected to provide temperatures high enough for the auto ignition of hydrogen to occur

without requiring a very heavy design for structural constraints. Same value $CR = 22:1$ was adopted in [12] for auto ignition of hydrogen in air.

With the amounts of hydrogen and oxygen and water proposed later, this selection of CR permits acceptable maximum pressures within the cylinder with temperatures at the start of injection well above the auto ignition temperature of hydrogen in air.

The auto ignition temperature of hydrogen in air is 860 K [12], which is significantly higher than the 520 K of conventional Diesel fuel. A requirement for a final compression temperature of at least 1100 K was proposed in [12] in order to achieve ignition delay below 1 ms of hydrogen in air. In the present application, oxygen and hydrogen are injected in the bulk of the combustion chamber surrounded by steam close to a continuously operating glow plug having a temperature in excess of 1300 K. Carefully shaping the injection profile of the cold oxygen and hydrogen should produce a diffusion controlled combustion following the kinetics controlled auto ignition.

The combustion is modelled through a simple Wiebe function with constant timing for 50% and duration 10%–90% in fuel mass burned for sake of simplicity. This is the most critical assumption of the simulations, because it is certainly true that the auto ignition of oxygen and hydrogen may occurs quickly in high temperature gases, and then the combustion of hydrogen and oxygen may rapidly evolve in the premixed reactants and then continues in the further reactants being mixed almost instantaneously after mixing, but exploring with the engine performance simulation software all the possible opportunities for timings and durations of water, hydrogen and oxygen injections, it is certainly possible to experience also points of quite different behaviours because of temperatures falling below the requested values and auto ignition having larger delays and eventually becoming impossible.

A coupled STAR-CCM [8] and DARS [9] complete simulation of the two strokes including the exhaust gas removal through the exhaust valves and the independent injection of oxygen and hydrogen gases and liquid water within the cylinder plus vaporization and combustion is certainly a much better way to explore the operation of this novel engine before the prototype testing could occur. However, while this approach requires significant computational efforts, some phenomena still requiring proper modelling still leave significantly large margins of uncertainty.

The friction mean effective pressure is computed through the Chen–Flynn correlation [10] with standard coefficients, while the indicated mean effective pressure is computed by the model. The power turbine is connected through a shaft and a gear to the crank train and supplements the torque production by the piston work.

The combustion chamber of this engine is a flat head, bowl-in-piston combustion chamber typical of direct injection Diesel engines. The jet ignition device is centrally located and all of the injectors are located nearby to inject the oxygen, hydrogen and water towards the centre of the bowl.

The temperatures of cylinder head, piston and cylinder bore are imposed in the wall temperature object, while the Woschni [10] correlation is used to represent the heat transfer.

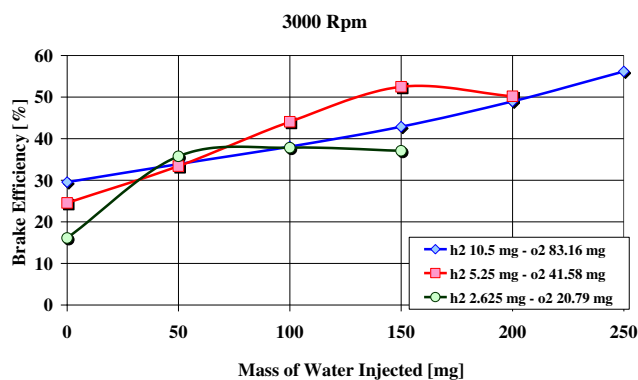


Fig. 2 – Brake fuel conversion efficiency at 3000 rpm with different masses of water, oxygen and hydrogen injected.

A simple Wiebe [10] function is used to represent the combustion evolution with imposed shape and duration parameters.

Because the water is injected liquid after combustion and there is no option to vaporize all the water when the combustion takes place, an evaporation object is added. This object prescribes the 50% evaporation duration and exponents for temperature and engine speed dependence. The amount of water injected that vaporizes immediately after injection may also be prescribed, leaving the evaporation object to model the remaining evaporation process.

In the cases considered below, the speed of the engine is 3000 Rpm. Injection of hydrogen is supposed to occur in 15° crank angle and it starts 5° crank angle before top dead centre. Injection of oxygen is also supposed to occur in 15° crank angle, but it starts 10° crank angle before top dead centre.

The exhaust valves having a diameter of 30 mm are open for 73° crank angle, with the maximum lift of 5 mm and the maximum lift crank angle of 145° before top dead centre.

Carefully shaping the injection profile for oxygen and hydrogen, combustion is supposed to occur with a 10–90% mass fuel burned of 5° crank angle and a 50% mass fuel burned located 5° crank angle after TDC.

Water is injected only during the expansion stroke in different quantities starting 30° crank angle before bottom

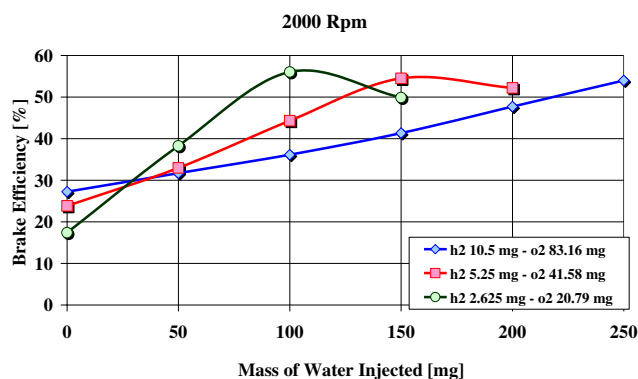


Fig. 3 – Brake fuel conversion efficiency at 2000 rpm with different masses of water, oxygen and hydrogen injected.

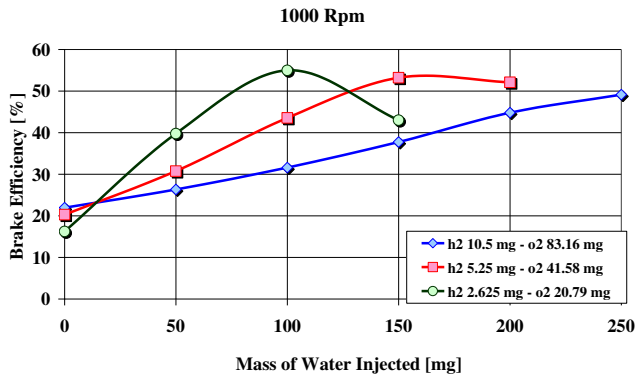


Fig. 4 – Brake fuel conversion efficiency at 1000 rpm with different masses of water, oxygen and hydrogen injected.

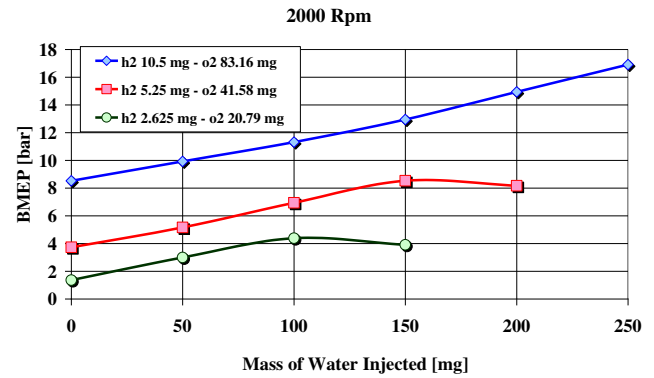


Fig. 6 – BMEP at 2000 rpm with different masses of water, oxygen and hydrogen injected.

dead centre. This may be too late under some conditions, because the peak cylinder temperature due to oxygen combustion is already over at this point where metal overheating might have occurred.

Figs. 2–7 presents the computed brake efficiency and brake mean effective pressure BMEP for operation at 3000, 2000 and 1000 rpm with different values of mass of water, oxygen and hydrogen injected.

All the events defined so far are a first guess of operating parameters and not optimized parameters. The relative amounts of water and oxygen and hydrogen, as well as the optimum timings for the start of the injections, the duration of the injection processes, the flow rates during the injection processes and the timings and openings of the exhaust are just first attempt values. Working with the specific hardware, these details might be subject to major revisions.

Even without water injection, the particular exhaust valve opening produces a significant amount of residuals. Injection of oxygen and hydrogen about top dead centre obviously increase the mass within the cylinder, as the injection of water before bottom dead centre also does. Increasing the amount of water injected obviously also increases the amount of residual gases trapped within the cylinder.

The injection of cold oxygen and hydrogen about top dead centre produces a drop in averaged temperatures before the

start of combustion. Auto ignition without water injection does not seem an issue, because the temperatures are very high. Increasing the amount of water injected, the temperature at the start of combustion reduces and auto ignition may eventually finally become impossible even when supported by a hot glow plug. For all the operating point considered, the temperature of the oxygen and hydrogen following their mixing close to the continuously operating glow plug at the centre of the chamber permits ignition delays below 1 ms (temperatures above 1100 K). Ideally, a pilot injection of hydrogen and oxygen should occur before the main oxygen and hydrogen injection in hot reacting gases.

Interesting to note the effect of the water injection on the exhaust gases trapped within the cylinder, with the mass of exhaust gases trapped at the end of the exhaust stroke much larger than the fresh oxygen and hydrogen introduced within the cylinder.

No optimization has been carried out on the model. The proposed parameters are therefore not the best choice. These preliminary results may be considered quite promising, with significant margins still left to achieve better brake mean effective pressures and/or brake engine thermal efficiencies following optimization of the injection events and of the fully variable actuation of the exhaust valves. However, the

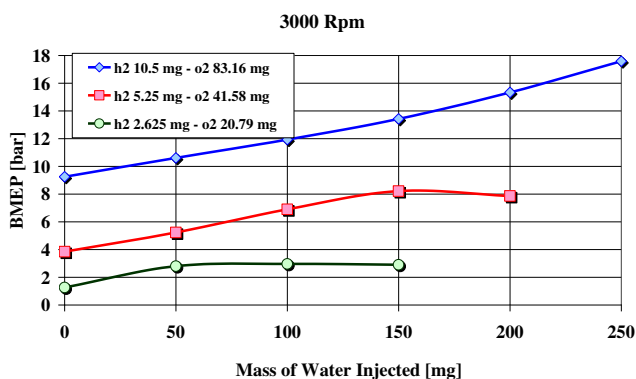


Fig. 5 – BMEP at 3000 rpm with different masses of water, oxygen and hydrogen injected.

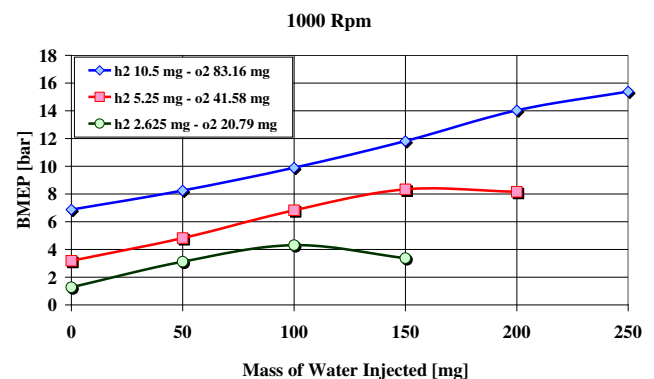


Fig. 7 – BMEP at 1000 rpm with different masses of water, oxygen and hydrogen injected.

inadequate modelling of injection, mixing and combustion does not suggest moving further the optimization.

Considering the application is not conventional, the next step will be to design a prototype engine following the proposed guidelines using the off-the-shelf components for the oxygen, hydrogen and water injectors and the power turbine together with specially manufactured single cylinder engine and the jet ignition device for a proper experimental proof of concept as well as the further refinement of the numerical model to better consider the many processes so far represented in a very simple way.

4. Conclusions

The hydrogen economy requires hydrogen as an energy carrier to be produced by renewable energy sources through the splitting of the water molecule. From this splitting, oxygen is a by-product that possibly could come with the hydrogen to permit internal combustion engines having very large efficiencies and power densities.

Hydrogen-oxygen internal combustion engines have to face the extreme temperatures resulting from the stoichiometric combustion of hydrogen in oxygen. The smart option to design an engine is to manage the steam produced during combustion recirculating the exhaust gases and producing steam injecting water.

In hypothesis to have oxygen and hydrogen available at high pressure, then a two stroke engine may be designed with direct injectors for water, hydrogen and oxygen and a fully variable exhaust valve actuation. Jet ignition may replace the spark plug to better ensure occurrence of a complete combustion. The combustion chamber may be the classical combustion chamber of a Diesel with a flat head and a bowl-in-piston.

First numerical simulations already provide brake fuel conversion efficiencies above 50%. It seems reasonable to guess efficiencies of the fully optimised and developed engine approaching the 60% mark. These efficiencies are 20% higher than those of the state-of-the-art H₂ICEs designed for operation with air using the spark-ignition engine concept of the HylCE project [11] as well as of those projected of Diesel engines with exhaust energy recovery. Worth of mention is also the much higher power density.

The next step will be to design a prototype engine following the proposed guidelines for a proper experimental proof of concept and the further refinement of the numerical model to

better consider the many processes so far represented in a way very simple due to the unconventional nature of this engine.

This engine has the ability to produce no pollutant at all, nor the NO_x (there is no nitrogen), nor the CO or CO₂ (there is no carbon). It is very well known that a Diesel engine has much better cost to efficiency ratio than every other engine, and this is the reason the Diesel engine is the preferred platform for trucks worldwide and for cars in Europe. The reason to try something different from the Diesel comes from the environmental implications of the Diesel, not the cost to produce and use. Nevertheless, the proposed engine concept could be competitive if properly industrialized not requiring particularly complicated hardware or software to operate.

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